LA-UR -85-400

CONF-850610--14

LA-UR--85-400

DE85 006681

TITLE: A NEW SLAB GEOMETRY RADIATION TRANSPORT DIFFERENCING SCHEME

AUTHOR(S): E. W. LARSEN, J. E. MOREL, W. F. MILLER, JR.

SUBMITTED TO: Extended abstract to be presented at the annual meeting of the American Nuclear Society, June 9-14, 1985, Boston, Mass.

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

A NEW SLAB GEOMETRY RADIATION TRANSPORT DIFFERENCING SCHEME

E. W. Larsen, J. E. Morel, W. F. Miller, Jr.
Los Alamos National Laboratory
P.O. Box 1663, MS-B226
Los Alamos, New Mexico 87545

Summary

Considerable effort has been directed toward seeking an optimal spatial differencing scheme for the neutron transport equation.[1] This search led to a best scheme (using specific criteria to define "best"): the linear characteristic method. However, we have recently considered radiative transfer problems in which the same problem may have both optically thick and optically thin regions, with the maximum optical thicknesses being much greater than those generally encountered in neutron transport problems. Here we describe the important features of these radiative transfer problems and a new differencing scheme which seems to have many advantages for radiative transfer calculations relative to the older schemes.

In radiative transfer problems, positivity of the scalar flux is extremely important because the radiative transfer model is usually part of a large physics code, with the radiative transfer solution coupled to other physics models. A scheme which is guaranteed-positive would be extremely useful, due to the large number of negative fluxes which are otherwise encountered, even with the linear-characteristic method. The alternative of

using a negative flux fixup can lead to a deterioration of the diffusion-synthetic-acceleration schemes which otherwise provide rapidly converged solutions.[2]

Owing to the presence of scattering regions that are optically thick, radiative transfer problems require a scheme that has the diffusion limit. By this we mean that as the problem becomes more diffusion-like (i.e., many mean-free-paths thick with scattering ratios very close to one and spatialy slowly-varying inhomogeneous sources), the transport differencing scheme explicitly becomes a diffusion differencing scheme. Although there is really only one diffusion limit for the analytic transport equation, there are several diffusion limits of interest for differenced forms of the transport equation. For instance, Larsen has described one particular limit in which an optically thick system is obtained by fixing the cell width and cross-sections and adding more cells.[3] Alternatively, one might fix the cell width and the number of cells and increase the cross-sections.

Thus, considering the characteristics of radiative transfer problems, we seek a scheme with the following properties:

1. Accuracy. The scheme satisfies particle balance, has the infinite-medium solution, $\psi = Q/\sigma_a$, and is second-order accurate as $\Delta x \to 0$.
2. Positivity. The scheme gives a guarenteed nonnegative solution for the cell-averaged scalar fluxes without the use of artificial fixups.
3. Diffusion Limit. The scheme has the diffusion limit for thick regions composed of thick cells (the "strong" diffusion limit). If possible, the scheme should also have the diffusion limit for thick regions composed of many thin cells (the "weak" diffusion limit).

The standard differencing schemes do not satisfy all these criteria. For example, the diamond scheme is not positive and does not satisfy the strong diffusion limit. The step characteristic method does not satisfy either diffusion limit. The linear characteristic method is not positive, and the Lund[4] method does not satisfy the accuracy requirements.

To begin our derivation of the new scheme, we require that it satisfy the balance equation:

$$\frac{\pm 1}{\epsilon_{m,i}} (\psi^{\pm}_{m,i+1/2} - \psi^{\pm}_{m,i-1/2}) + \psi^{\pm}_{m,i} = c_i \phi_i + \frac{Q_i}{\sigma_{t,i}} \quad , \tag{1}$$

where ψ^+_m and ψ^-_m refer to fluxes traveling in the positive-μ and negative-μ directions respectively for a fixed $|\mu_m|$, $\epsilon_{m,i} = \sigma_{t,i}\Delta x_i/|\mu_m|$, $c_i = \sigma_{si}/\sigma_{ti}$, and we have assumed isotropic scattering and sources. Note that for an infinite medium:

$$\psi_{m,i+1/2} = \psi_{m,i-1/2} = \psi_{m,i} = \phi_i = \frac{Q_i}{\sigma_{a,i}} \quad .$$

An auxilliary equation is needed with Eq.(1) because there are two unknowns (the right side is known from the previous iteration): the exiting and cell-average angular fluxes. We select an auxilliary equation of the form:

$$\begin{aligned} \psi^{\pm}_{m,i} = \gamma_{m,i}\psi^{\pm}_{m,i\pm 1/2} + (1 - \gamma_{m,i})\, 0.5\, (\psi^{+}_{m,i\pm 1/2} + \psi^{-}_{m,i\pm 1/2}) \\ + \rho_{m,i}(\psi^{\pm}_{m,i\mp 1/2} - \psi^{\pm}_{m,i\pm 1/2}) \quad , \end{aligned} \tag{2}$$

which, depending on the definition of $\gamma_{m,i}$ and $\rho_{m,i}$, defines a class of methods, all of which allow the infinite-medium solution.

To obtain a condition for positivity, we eliminate $\psi^{\pm}_{m,i}$ between Eqs. (1) and (2), yielding explicit formulas for the exiting edge angular fluxes in terms of the entering edge angular fluxes and the scattering and inhomogeneous sources. Requiring these exiting fluxes to be non-negative, we obtain the bounds:

$$1 \geq \varepsilon_{m,i}\rho_{m,i} \,, \tag{3a}$$

$$1 + \gamma_{m,i} \geq 2\rho_{m,i} \,, \tag{3b}$$

$$\gamma_{m,i} \geq 1 \,. \tag{3c}$$

Then by properly manipulating the available equations, and using the relationship:

$$\phi_i = \sum_{\mu_m > 0} \psi^{+}_{m,i}\, w_m + \sum_{\mu_m < 0} \psi^{-}_{m,i}\, w_m \,,$$

we find that Eqs. (3) assure a nonnegative cell-average scalar flux. Thus for each cell, if the entering angular fluxes and sources are nonnegative, the exiting angular fluxes and cell-average scalar fluxes will be nonnegative. The individual cell-average angular fluxes are not guaranteed to be positive, but these quantities are not used after the cell is calculated, and hence the their signs are irrelevant.

Next, a simple error analysis shows that to achieve second-order accuracy, we must have (for small $\varepsilon_{m,i}$):

$$\gamma_{m,i} = 1 + O(\varepsilon^{2}_{m,i}) \,, \tag{4a}$$

$$\rho_{m,i} = 0.5 + O(\varepsilon_{m,i}) \,, \tag{4b}$$

To show the strong diffusion limit, for a small parameter δ, we let:

$$\sigma_t \rightarrow \frac{\sigma_t}{\delta} , \tag{5a}$$

$$c \rightarrow 1 + \delta^2 (c - 1) , \tag{5b}$$

$$Q \rightarrow \delta Q . \tag{5c}$$

Then we require that the transport differencing scheme become a differencing scheme for the diffusion equation in the limit as $\delta \rightarrow 0$. An analysis shows that this occurs if:

$$\gamma_m = 0.5\varepsilon_m + O(1) , \tag{6a}$$

$$\rho_m = O(\frac{1}{\varepsilon_m}) , \tag{6b}$$

A particular method which satisfies Eqs. (3), (4), and (6) is defined by:

$$\rho_{m,i} = \frac{1 - \exp(-\varepsilon_{m,i})(1 + \varepsilon_{m,i})}{\varepsilon_{m,i}(1 - \exp(-\varepsilon_{m,i}))} , \tag{7a}$$

$$\gamma_{m,i} = 1 + c_i\varepsilon_{m,i}(0.5 - \rho_{m,i}) . \tag{7b}$$

This selection of $\gamma_{m,i}$ and $\rho_{m,i}$ also assures the exact solution for $c = 0$ with a uniform inhomogeneous source, and the weak diffusion limit.[3]

We have solved a sample problem with this new scheme, the standard diamond scheme, and the Lund scheme. The problem consists of a uniform 10 cm-thick slab with $\sigma_t = 1.0\ \text{cm}^{-1}$ and $c = 0.5$, an isotropic flux with unit current incident on the left face, zero incident flux on the right face, and ten uniform spatial cells, each having a thickness of one mean-free-path. The cell-average scalar fluxes are plotted in the figure, and we see that the new method gives a solution which is almost indistinguishable from the exact solution, and clearly outperforms both the diamond and Lund schemes. Note that the point value for the diamond solution at x = 0.95 could not be included in the semi-log plot because it is negative.

Acknowledgement

This work was performed under the auspices of the U. S. Department of Energy.

References

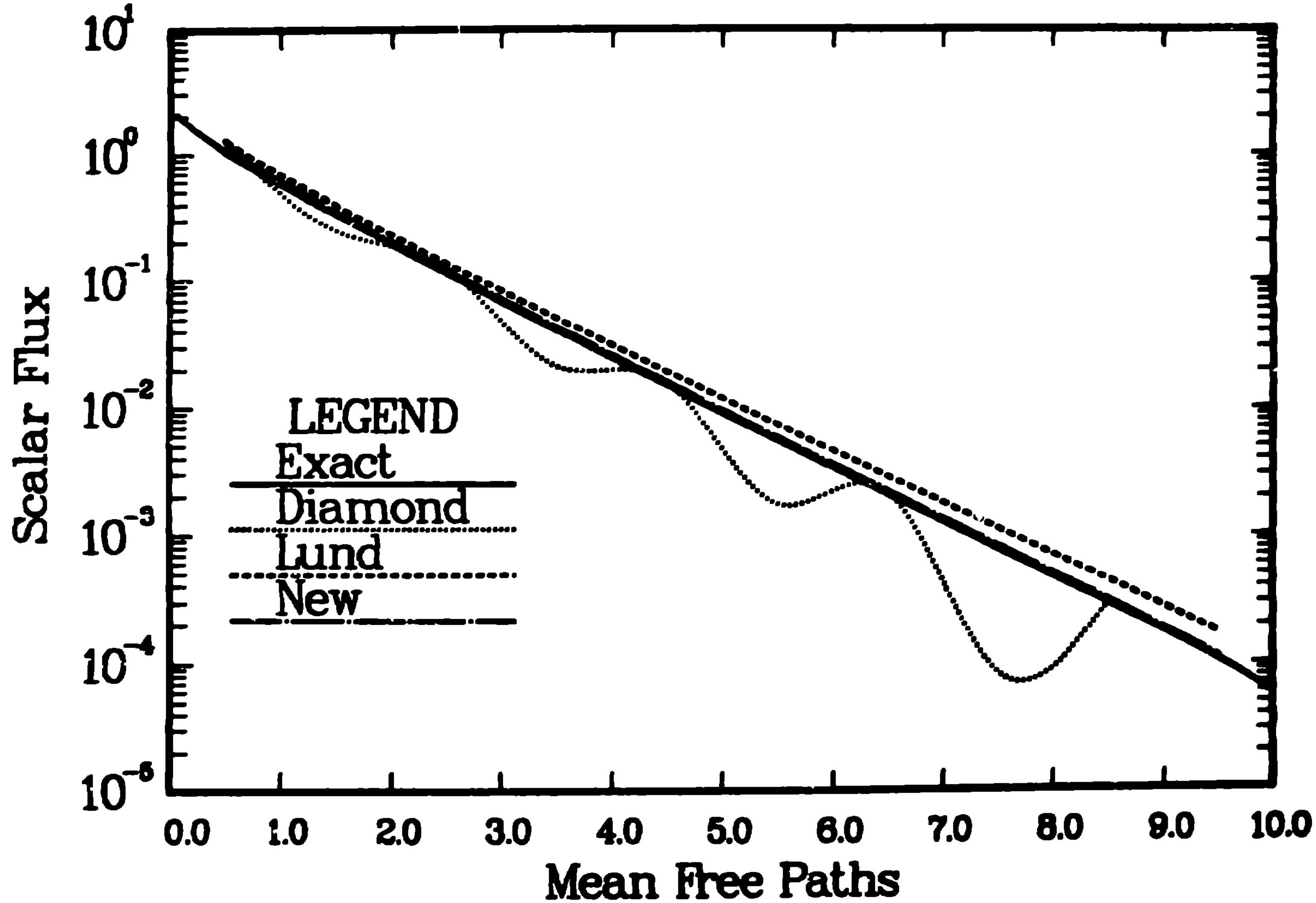
1. R. E. Alcouffe, E. W. Larsen, W. F. Miller, Jr., and B. R. Wienke, Nucl. Sci. Eng., 71, 111 (1979).

2. D. R. McCoy and E. W. Larsen, Nucl. Sci Eng., 82, 64 (1982).

3. E. W. Larsen, Nucl. Sci. Eng., 83, 90 (1983).

4. C. M. Lund, "Radiation Transport in Numerical Astrophysics," UCRL-88720, Lawrence Livermore National Laboratory report (1983).

Figure Caption: Scalar Flux Comparison for Sample Problem.



10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Scalar Flux
LEGEND
Exact
Diamond
Lund
New
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
Mean Free Paths